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On the sensitivity of He I singlet lines to the Fe IV model atom in O stars

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ABSTRACT

Aims. Recent calculations and analyses of O star spectra have revealed discrepancies between theory and observations, and between different theoretical calculations, for the strength of optical He I singlet transitions. We investigate the source of these discrepancies.
Methods. Using a non-LTE radiative transfer code we have undertaken detailed test calculations for a range of O star properties. Our principal test model has parameters similar to those of the O9V star, 10 Lac.
Results. We show that the discrepancies arise from uncertainties in the radiation field in the He I $1s^2\,{}^1S$–$1s\,2p\,{}^1P^\circ$ transition near 584 Å. The radiation field at 584 Å is influenced by model assumptions, such as the treatment of line-blanketing and the adopted turbulent velocity, and by the Fe IV atomic data. It is shown that two Fe IV transitions near 584 Å can have a substantial influence on the strength of the He I singlet transitions.
Conclusions. Because of the difficulty of modeling the He I singlet lines, particularly in stars with solar metalicity, the He I triplet lines should be preferred in spectral analyses. These lines are much less sensitive to model assumptions.

Key words. stars: atmospheres – stars: early-type – line: formation – radiative transfer

1. Introduction

With the advent of non-LTE line-blanketed model atmosphere calculations (Hubeny & Lanz 1995; Hillier & Miller 1998; Pauldrach et al. 2001; Gräfener et al. 2002; Puls et al. 2005) considerable advances in the analysis of massive stars have been made. There has, for example, been a significant downward revision in the effective temperature of O stars (Martins et al. 2002, 2005a; Crowther et al. 2002; Herrero et al. 2002; Bianchi & Garcia 2002; Garcia & Bianchi 2004; Repolust et al. 2004; Massey et al. 2004, 2005). Moreover, the discrepancy between spectroscopic and evolutionary masses (Groenewegen et al. 1989; Herrero et al. 1992) has been greatly reduced (e.g., Herrero 2003; Repolust 2004).

A key diagnostic of the effective temperature in O stars is the ratio of He I line strengths relative to those of He II (e.g., Kudritzki et al. 1983; Herrero et al. 2000). However detailed comparisons with observations show discrepancies larger than expected. Further, theoretical modeling reveals sensitivities of some lines to the adopted techniques and assumptions while there are also discrepancies between results obtained using different codes.

From very early on it was realized that in extended atmospheres the $1s\,2p\,{}^3P^\circ$ and $1s\,2p\,{}^1P^\circ$ states become overpopulated, and that this affects the strength of the He I lines (e.g., Wellmann 1952a,b,c; Ghobros 1962). This is termed the dilution effect, and was more recently discussed by Voels et al. (1989). With the advent of non-LTE line-blanketed model atmospheres it was expected that the new model atmospheres would be capable of modeling the full He I spectrum. However, as noted by Hillier et al. (2003), it was not possible to get a simultaneous fit to all He I lines. Further, in that study of two O stars in the SMC, it was noted that the He I singlet lines were more sensitive to model details than the He I triplet line 4473 Å (vacuum). As additional studies have been undertaken it has become clear that while model calculations often have difficulty fitting the He I singlet transitions they give satisfactory fits for the He I triplet lines (e.g., Puls et al. 2005; Repolust et al. 2005; Martins et al. 2005b; Massey et al. 2005; Mokiem et al. 2005; Lanz et al. 2006).

More recently, comparisons between CMFGEN (Hillier & Miller 1998) and TLUSTY (Hubeny & Lanz 1995), and between CMFGEN and FASTWIND (Puls et al. 2005), have shown inconsistent predictions, in some parameter ranges, for the strength of the He I singlet lines (e.g., Puls et al. 2005). The disagreement between CMFGEN and TLUSTY was somewhat surprising since previous comparisons (e.g., Hillier & Lanz 2001; Bouret et al. 2003) had shown excellent agreement. However the comparisons were limited to a few models, and it is has become apparent that the discrepancies only occur for certain parameter ranges. Given the different assumptions in the codes, different atomic data, and different techniques, it is not immediately obvious which code is giving the correct answers. Agreement between observations and CMFGEN was improved in some cases, for example, by adding additional species (e.g., argon, neon, nickel and calcium), and by reducing the turbulent velocity used in the atmospheric structure/population calculations from 20 to 10 km s^{-1} (Martins et al. 2005b).

Table 1. Atomic data.

Ion	Low level[1]	Upper level	λ(Å)	ΔV (km s^{-1})[2]	A_{ul}	f^3_{lu}	f^4_{lu}
He I	1s 2s ^{1}S	1s 2p ^{1}P°	20586.9		1.73×10^6	0.329	
He I	1s^2 ^{1}S	1s 2p ^{1}P°	584.334		1.78×10^9	0.274	
Fe IV	3d^5 ^{4}F$_{9/2}$	3d^4(^{3}G)4p ^{2}H$^\circ_{9/2}$	584.368	17	6.82×10^7	0.00349	0.00251
Fe IV	3d^5 ^{2}D3$_{5/2}$	3d^4(^{3}G)4p ^{4}H$^\circ_{7/2}$	584.397	32	4.22×10^8	0.0288	0.00264

[1] Level designations for Fe IV are from the NIST Atomic Spectra Database. The D3 designation is used to denote one of the three 3d^5 ^{2}D terms; [2] velocity shift of Fe IV transition relative to He I λ584 transition; [3] Fe IV oscillator strengths are from Kurucz & Bell (1995); [4] Fe IV oscillator strengths are from Becker & Butler (1995).

In this paper we discuss the analysis of He I lines in O stars, and the inconsistencies between triplet and singlet lines, between observations and models, and between results obtained using different atmospheric codes. The complicated behavior of the He I singlet line strengths is shown to be a consequence of complicated radiative transfer effects in the neighborhood of the He I 1s^2 ^{1}S–1s 2p ^{1}P° transition at 584 Å. In particular, it is shown that two Fe IV lines, which closely coincide in wavelength with this transition influence the population of the 1s 2p ^{1}P° level, and thus the strength of He I singlet lines that couple to the 1s 2p ^{1}P° level. Indeed, a closer examination of the discrepancies reveals that the lines that are most discordant between different model calculations are not the He I singlet lines per se, but rather the transitions involving 1s 2p ^{1}P°.

That line-line interactions, and the precise details of line blanketing in the far UV, might affect optical line diagnostics is not surprising. In planetary nebula the fluorescence of O III lines by He II Lyα (the Bowen mechanism, Bowen 1934) is well documented (see, e.g., Osterbrock 1989). In WN stars many of the N lines are affected by continuum fluorescence processes, and hence sensitive to blanketing (Hillier 1988). Further, Schmutz (1997) suggested that photon loss from the He II resonance transition, by overlapping metal lines, could significantly affect the ionization structure in W-R stars and hence help to solve the problem of how to accelerate W-R winds. The effect was investigated in modeling the WC component of the WR+O binary γ Velorum (De Marco 2000), and found to be important. Martins (2004) investigated the same mechanism in O star models (i.e., the influence of metal lines near He II Lyα) and also found that the effects were significant.

2. The interaction of He I with Fe IV

A simplified Grotrian diagram for the He I atom (singlets only) is shown in Fig. 1. For the present discussion the most important transition is the 1s^2 ^{1}S–1s 2p ^{1}P° transition at 584 Å. Key transitions, often used for diagnostic purposes, are indicated. Overlapping the 584 Å transition are several Fe IV transitions. The data for the relevant Fe IV transitions used in CMFGEN, taken from Kurucz & Bell (1995), is provided in Table 1 – only the two most important transitions are shown. Wavelengths for the Fe IV transitions were calculated using the known energy levels given in the NIST Atomic Spectra Database (`http://physics.nist.gov/PhysRefData/ASD/index.html`), and are believed to be accurate[1]. The velocity separation of the two Fe IV lines from the HeI λ584 is given, as are the oscillator strengths computed by Becker & Butler (1995). These show significant differences to those of Kurucz & Bell (1995), and indicate that the oscillator strengths for these transitions must be regarded as uncertain.

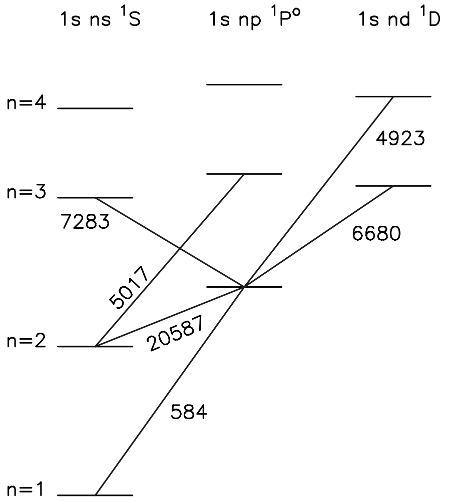

Fig. 1. Simplified Grotrian diagram for the singlet states of He I. The λ584 transition plays a key role in determining the population of the 1s 2p ^{1}P° level, and hence the strength of transitions that involve that level. Although not shown, another important line often used as a diagnostic (λ4389; 1s 2p ^{1}P°–1s 5d ^{1}D) also involves the 1s 2p ^{1}P° state.

In O stars He I 584 Å is often optically thick, so that photons undergo a number of scatterings within the line before escaping. Because the optical depth is large, a high population of the 1s 2p ^{1}P° state is maintained enhancing the strength of absorption lines ending on this state. However, as the photons scatter other mechanisms come into play. In particular, they can be absorbed by the overlapping Fe IV lines. As the upper states of these levels have alternative decay routes, the absorbed photons can be removed from the 584 transition, acting as a drain, and causing the 1s 2p ^{1}P° population to be lowered. This leads to a weakening of the transitions whose lower state is 1s 2p ^{1}P°. Clearly the importance of this effect in model atmosphere calculations will depend on whether the explicit interaction between the He I resonance transition and the Fe IV lines is taken into account, the accuracy of the Fe IV wavelengths, oscillator strengths and branching ratios, and on other atmospheric parameters such as the adopted microturbulent velocity. It is also obvious that the importance of the effect will depend on the actual stellar parameters (i.e., $T_{\rm eff}$, $\log g$, $\dot{M}$).

In this study we concentrate specifically on the influence of the two Fe IV lines on the He I line strengths. It should be

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[1] The energy values for the relevant lower levels in the NIST table are quoted to 0.1 cm^{-1}, while the upper levels are quoted to an accuracy of 0.01 cm^{-1}. An accuracy of 0.1 cm^{-1} in the energy difference between the two levels corresponds to less than 0.2 km s^{-1}, and thus it is unlikely that the wavelengths are significantly in error.

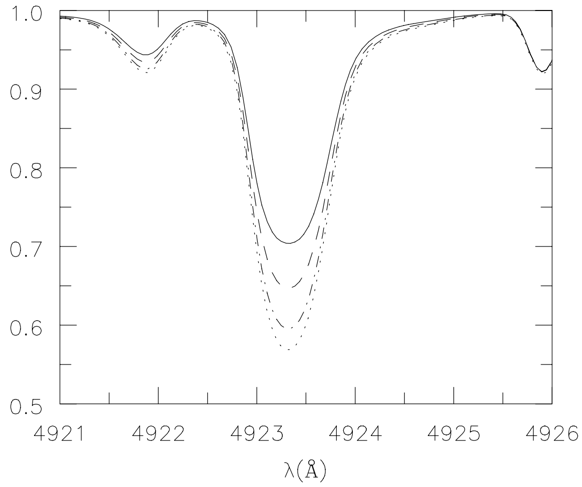

Fig. 2. Predicted line profiles for He I λ4923 (2p ^{1}P°–4d ^{1}D). The solid curve shows the prediction with the standard model, while the other curves show the profiles when the relevant Fe IV f values are reduced by a factor of 2 (dashed curve), a factor of 5 (dot-dash), and a factor of 10 (dot).

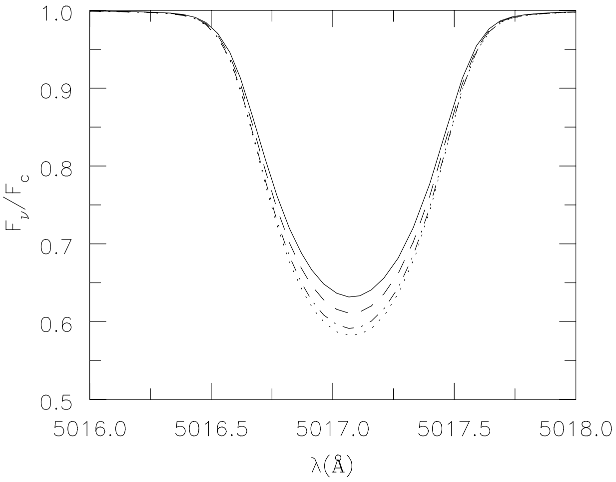

Fig. 3. As for Fig. 2 but for He I λ5017 (1s 2s ^{1}S–1s 3p ^{1}P°). The line strengths have changed significantly, but the change is less than for transitions ending on 1s 2p ^{1}P°.

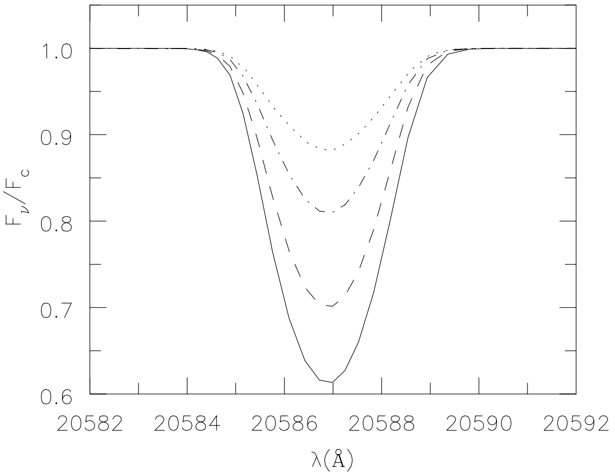

Fig. 4. As for Fig. 2 but for He I λ20587 (2s ^{1}S–2p ^{1}P°). Because the 1s 2p ^{1}P° state is the upper level of this transition, the variations in the strength are in the opposite sense to the optical lines.

stressed, however, that other Fe IV lines, and lines due to other species (e.g., Ca V, Fe VI) could also potentially have an influence (albeit generally weaker) on the He I singlet line strengths.

3. Results

In order to quantitatively explore the influence of the Fe IV lines on the He I lines we consider the following model: $T_{\rm eff}$ = 33 560 K, $\log g$ = 3.9, $L = 7.13 \times 10^4\ L_\odot$, $R_* = 7.8\ R_\odot$, $\dot{M} = 1.0 \times 10^{-8}\ M_\odot\ {\rm yr}^{-1}$, $V_\infty = 1400\ {\rm km\,s}^{-1}$. The parameters of the model are similar to models we are using to investigate the O9V star 10 Lac (Lanz et al. 2006). Since the mass-loss is low, the important parameters for the present study are $T_{\rm eff}$ and $\log g$ only. The hydrostatic structure was initially obtained from a TLUSTY model but has been subsequently modified as the parameters were changed. Below 5 km s^{-1} hydrostatic equilibrium is achieved to generally better than 5%. Unless otherwise stated, we used a fixed Doppler width of 13.5 km s^{-1} in the atmosphere calculations, while a turbulent velocity of 10 km s^{-1} was adopted for the profile calculations. The N(He)/N(H) ratio is taken as 0.1 while we adopted solar abundances using the compilation of Grevesse & Saval (1998). CNO abundances were reduced slightly in accord with the recent results by Asplund et al. (2005).

3.1. *He I singlet sensitivities: f values, abundances, and turbulent velocities*

In order to test the sensitivity of the models to the oscillator strengths of the two relevant Fe IV transitions we ran a detailed CMFGEN model using the tabulated f values, and then models in which the f values were reduced by factors of 2, 5, and 10. The results for He I λ4923, λ5017, λ20587, and λ4473, are shown in Figs. 2–5 respectively. The three singlet lines show significant variations. For the transition with 1s 2p ^{1}P° as the lower level, the line is strongest in the model with the lowest f values. As noted earlier Fe IV transitions drain photons from the 1s^2 ^{1}S–1s 2p ^{1}P° transition, lowering the equilibrium 1s 2p ^{1}P° population. When the oscillator strength is lowered the drain is weakened, and the 1s 2p ^{1}P° population is enhanced. The λ4923 transition, which is coupled directly to the 1s 2p ^{1}P° state, shows a large variation (Fig. 2), while the λ5017 line (Fig. 3), which has 2s ^{1}S as its lower state, shows smaller variations. Another transition, He I λ6680, which also has 1s 2p ^{1}P° as its lower state, shows similar or even more sensitive behavior than λ4923. The near IR transition, He I λ20587 (1s 2s ^{1}S–1s 2p ^{1}P°), also shows very significant variations. However, in this case, the absorption profiles are strongest when the f values are largest. This is to be expected, since for this transition the 1s 2p ^{1}P° state is the upper level. The difficulty in modeling the λ20587 line in early type stars has been discussed extensively, for example, by Najarro et al. (1994). The problem with λ20587 has not been fully solved with models accounting for blanketing. In their analysis of WR147, Morris et al. (2000) found that this line was one of the very few lines for which a discrepancy still appeared. They obtained a much too deep He I 20587 line, consistent with the singlet problem presented here. The He I λ20587 line is very important for analyses of O stars using H and K band infrared data (Repolust et al. 2005), and hence it is important that its formation be understood.

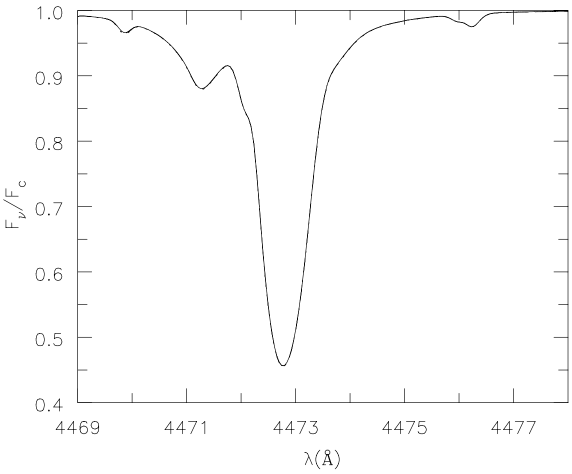

Fig. 5. As for Fig. 2 but for He I λ4473 (2p ^{3}P°–4s ^{3}D). The triplet line strengths are not affected by changes in the Fe IV line strengths.

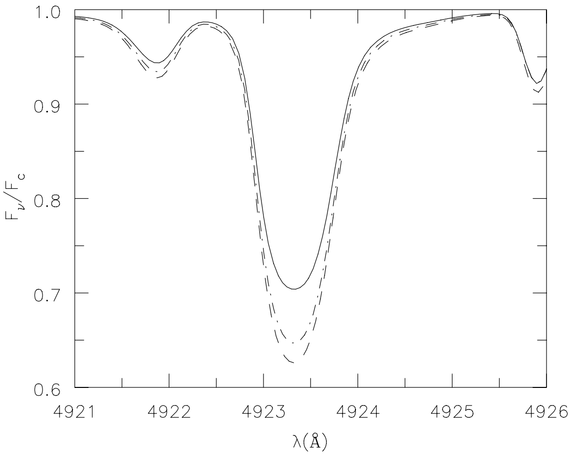

Fig. 6. Predicted line profiles for He I λ4923 (2p ^{1}P°–4d ^{1}D). The solid curve shows the prediction with the standard model, the dashed curve for a factor of 2 reduction in the Fe abundance, and the dot-dash curve for a factor of 2 reduction in the relevant Fe IV f values.

The triplet line, He I λ4473, is essentially identical in the 4 models (Fig. 5). Similar statements also apply to other He I triplet lines (e.g., λ5877). Limited tests with TLUSTY and FASTWIND confirm the changes found using CMFGEN.

Another obvious way to reduce the "drain" is to lower the Fe abundance. Indeed, as seen from Fig. 6, a reduction in the Fe abundance by a factor of 2 gives a similar enhancement in line strength in λ4923 as does the factor of 2 reduction in the Fe line strengths. The correspondence is not exact since a lower Fe abundance reduces line blanketing and hence causes slight changes in the temperature structure of the model atmosphere. As before, the λ4473 profiles are very similar in the three models. The sensitivity of the singlet lines to the Fe abundance explains why Hillier & Lanz (2001) achieved excellent agreement when comparing models for SMC O stars where the Fe abundance is only 0.2 solar.

As a final test of the sensitivity of the He I line strengths we examined the effect of the microturbulent velocity used in the atmosphere structure calculations to determine the level populations. In Fig. 7 we show the profiles for λ4923 computed using the same turbulent velocity for the profile calculations (10 km s^{-1}) but computed using fixed Doppler widths of 10 and 13.5 km s^{-1} for the determination of the atomic populations. As might be expected, λ4923 is stronger when computed using the lower turbulent velocity. With the larger turbulent velocity there is better overlap between the Fe IV and the He I line, and hence a more effective drain.

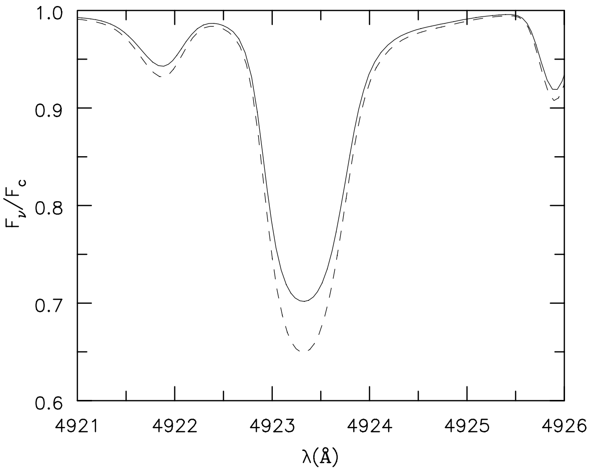

Fig. 7. Predicted line profiles for He I λ4923 (2p ^{1}P°–4d ^{1}D). The solid curve shows the prediction with the standard model while the dashed curve shows the effect of a lower turbulent velocity in the calculation of the level populations.

The use of 10 km s^{-1} for population calculations in O stars is not unusual. Detailed analyses suggest that this turbulent velocity is fairly typical, with possible lower values for dwarfs, and somewhat higher values for supergiants. The precise physical cause/meaning of microturbulent velocities derived from profile fitting is unclear.

We have also performed test calculations for other "typical" O star parameters. Similar effects are seen to occur, although the size of the changes depends strongly on spectral type. The mechanism does not appear to be operative for B stars, and in a model of a late O supergiant ($T_{\rm eff}$ = 28 400 K, $\log g$ = 3.2, $\dot{M}$ = 1.65 × 10^{-6} $M_\odot$ yr^{-1}, L = 5.4 × 10^5 $L_\odot$) the influence of the Fe IV lines was rather small, as illustrated in Fig. 8. Conversely, the influence in an early O dwarf ($T_{\rm eff}$ = 41 300 K, $\log g$ = 4.0, $\dot{M}$ = 2.0 × 10^{-6} $M_\odot$ yr^{-1}, L = 2.35 × 10^5 $L_\odot$), where the He I lines are weak, is relatively strong (Fig. 9). Interestingly, in a mid-O supergiant ($T_{\rm eff}$ = 36 200 K, $\log g$ = 4.0, $\dot{M}$ = 9.5 × 10^{-7} $M_\odot$ yr^{-1}, L = 2.35 × 10^5 $L_\odot$), a reduction of a factor of 10 in the two Fe IV oscillator strengths can cause He I λ4923 to change from being weakly in emission to a relatively strong absorption line.

In principle, f values could be empirically derived from a model comparison with observation. However, given the problem with turbulent velocities, and the sensitivities to the Fe abundance and other stellar parameters, we refrain from providing actual values. However, it does appear that both the Kurucz & Bell (1995) values, and the Becker & Butler (1995) values, are too large.

Taken as a whole, these findings explain the different results obtained between TLUSTY, CMFGEN, and FASTWIND. While TLUSTY and CMFGEN use similar data for Fe IV the models are not always computed using the same assumptions, such as which species are included and the adopted turbulent velocity. In CMFGEN, a smaller turbulent velocity leads to a longer computational time, and so a larger turbulent velocity is often adopted. In general the choice has very little effect of the population determinations but for a few lines, as shown here, the adopted

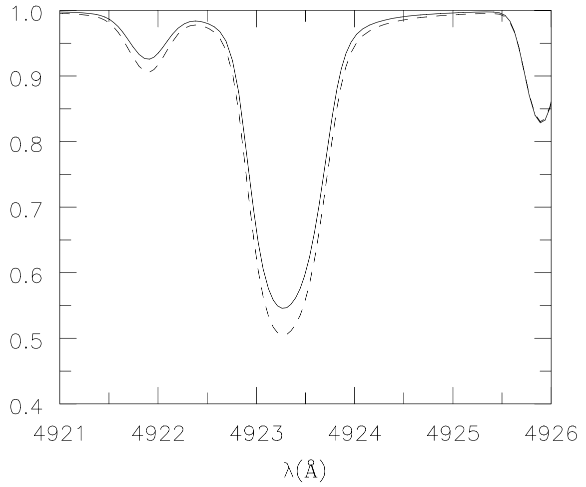

Fig. 8. Predicted line profiles for He I λ4923 (2p ^{1}P°–4d ^{1}D) in a model for a late O supergiant. The solid curve shows the prediction with the standard model, while the other curve shows the profile when the relevant Fe IV f values are reduced by a factor of 10.

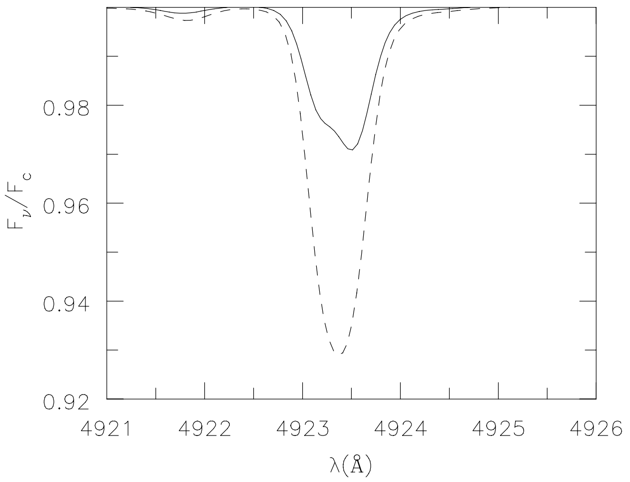

Fig. 9. Predicted line profiles for He I λ4923 (2p ^{1}P°–4d ^{1}D) in a model for an early O dwarf. The solid curve shows the prediction with the standard model, while the other curve shows the profile when the relevant Fe IV f values are reduced by a factor of 10.

value can be important. The adopted turbulent velocity was also shown to directly affect the He II λ4687 line in B supergiants (Evans et al. 2004). In FASTWIND blanketing is treated using mean opacities and emissivities, and consequently the detailed interaction between the 1s^2 ^{1}S–1s 2p ^{1}P° lines at 584 Å and the Fe IV lines is not taken into account, although work is in progress to rectify this. Since all three codes give similar answers for the He I triplet lines, the triplet lines are clearly preferred for spectral analyses.

As noted by the referee, Herrero et al. (2002) were able to obtain a good fit to the He I λ4473, and λ4389 lines using a model with $T_{\rm eff}$ = 35 500 ± 500 K and log g = 3.95 ± 0.1. This can be explained by noting that in 10 Lac it appears that the neglect of the influence of the two Fe IV transitions on the He I singlet transitions is a reasonable approximation. Finally, it should be noted that FASTWIND consistently gives temperatures, for O dwarfs, that are 1500 K higher than CMFGEN (and TLUSTY). The reason for the discrepancy is unknown but is being investigated. Mokiem et al. (2005) also obtained similar fit parameters to that of Herrero et al. ($T_{\rm eff}$ = 35 000 ± 850 K and log g = 4.03 ± 0.13) using numerous FASTWIND models and a sophisticated genetic algorithm. However, they derived a turbulent velocity of 15.5 ± 4 km s^{-1} which is inconsistent with that indicated by the metal lines (Lanz et al. 2006), again suggesting that possible systematic effects in the models are being neglected (see additional discussion in Lanz et al. 2006).

4. Conclusion

Earlier work on the analysis of massive O stars revealed inconsistencies in the predictions of He I line strengths with observations, and between different codes. We have shown that these inconsistencies arise because of the different treatment of line-blanketing in the neighborhood of the He I 1s^2 ^{1}S–1s 2p ^{1}P° transition at 584 Å, due to different treatments regarding the interaction of the He I and Fe IV model atoms, and due to different adopted model Fe IV atoms. The adopted microturbulent velocities and iron abundance also play a direct role in determining the population of the 1s 2p ^{1}P° state, and hence on the He I singlet line strengths.

The accurate prediction of He I lines, which involve 1s 2p ^{1}P°, is difficult, and possibly not feasible with the current atomic data available for Fe IV. We argue strongly that the He I triplet lines should be weighted the most heavily when performing spectral analyses. Inconsistencies between model fits of the He I singlet lines and triplet lines, and between those singlets connected to 1s 2p ^{1}P° (e.g., λ4923) and other singlet lines (e.g., λ5017; 1s 2s ^{1}S–1s 3p ^{1}P°) are indicative of significant transfer effects in He I λ584.

Extensive modeling by one of us (Najarro) suggests that the Kurucz Fe IV oscillator strengths are too large but given the uncertainties in the models, and the influence of the turbulent velocity, it is not feasible to determine reliable empirical values.

We have shown how subtle radiative transfer effects can significantly influence the strength of the He I singlet transitions. It is possible that similar effects may occur for other diagnostic lines, especially if the levels involved in such transitions are coupled to low lying levels whose population may be effected by overlap between strong transitions and metal lines.

Interestingly, the subtle effect of the Fe IV lines on the 1s 2p ^{1}P° population may contribute to the dilution effect. In early unblanketed O star models, triplet lines were consistently too weak compared with observations, especially in stars of class II, Ib, and Ia (Voels et al. 1989). This was interpreted as a problem with the triplet lines, and was believed to arise from the neglect of extension effects. Intriguingly, all the singlet lines analyzed by Voels et al. (1989) involve the 1s 2p ^{1}P° state. While it is now known that blanketing is much more important than was previously suspected, the use of spherical models, the allowance for stellar winds, and the influence of line blanketing (as in FASTWIND) has not alleviated the problem with He I λ4473 in giants and supergiants of type O6 and later (Massey et al. 2005; Repolust et al. 2004). Physically, and with the new generation of models, it is much easier to understand the inconsistencies in the He I line strengths as arising from problems in computing the population of the 1s 2p ^{1}P° state and hence the singlet line strengths, rather than the triplet line strengths.

This work highlights the importance of performing analyses with independent codes, and with performing systematic analyses of all available lines. In this way discrepancies, sensitivities, and biases can be determined and investigated. The work also highlights the importance of understanding the physics of line formation if one is to derive accurate abundances. This is especially true in situations where only one or two spectral lines are available for analysis – a situation not uncommon in O stars.

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